STRONG FIELD COHERENCE BREAKING AS A TOOL FOR IDENTIFYING ROTATIONAL TRANSITIONS DUE TO METHYL ROTOR STATES: 2-HEXANONE

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As energy demands increase, more sustainable alternatives to finite fossil fuels need to be explored. Ketones are an important constituent in biomass derived liquids and small methyl ketones have high octane numbers and show low emissions of soot, yet, their combustion chemistry remains relatively unexplored. 2-hexanone is an interesting candidate as it has a long alkyl chain supporting numerous conformational isomers as well as a methyl rotor. In this study, the rotational spectrum of 2-hexanone was recorded over the 8-18 GHz region using a chirped pulse Fourier transform microwave (CP-FTMW) spectrometer. Strong field coherence breaking (SFCB) was utilized to selectively modulate rotational transitions belonging to the two lowest energy conformers of 2-hexanone, aiding the assignment. In addition, the SFCB method was applied for the first time to identify rotational transitions built off the two lowest energy hindered methyl rotor states of each conformer, 0a1 and 1e. Since these two states have rotational energy levels with different nuclear spin symmetries, their intensities could be selectively modulated by the resonant monochromatic pulses used in the SFCB method. The difference spectra, final fit and structural parameters will be discussed for all three conformers assigned.